

Gweicurculactone
123914-43-2 | DTXSID50154143

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 318 °C

Global applicability domain: Inside

Local applicability domain index: 4.46e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

Image not found

Phosphine, ethyldiphenyl-

Measured: 293

Predicted: 310

Image not found

4-Bromobenzophenone

Measured: 350

Predicted: 336

Image not found

4-Methoxybenzophenone

Measured: 355

Predicted: 329

Image not found

4-Chlorobenzophenone

Measured: 332

Predicted: 320